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ScienceDirect

Acta Materialia 91 (2015) 330–339

Acta MATERIALIA

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Ordered α_2 to ω_o phase transformations in high Nb-containing TiAl alloys

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Received 6 January 2015; revised 11 March 2015; accepted 12 March 2015
Available online 2 April 2015

Abstract—The transformation of the $D0_{19}$-α_2 phase to the $B8_2$-ω_o phase is a new type of phase transformation in high Nb-containing TiAl alloys; experimental results concerning this phase transformation are still lacking. Moreover, studies on the orientation relationships (ORs) between these two phases are scarce compared with those reported between the disordered ω and α phases, which can be more complicated due to their ordered structures. In this study, the direct α_2 to ω_o phase transformation is observed by transmission electron microscopy (TEM) and high-resolution transmission electron microscopy (HRTEM). The ω_o phase is transformed from the α_2 laths in the lamellar structure after annealing over long periods at 850 °C. The various ORs observed between these two phases can be merged into two typical ORs: $[11\bar{2}0]_{\alpha2}//[0001]_{\omega o}, (0002)_{\alpha2}//(11\bar{2}0)_{\omega o}$ and $[1\bar{1}00]_{\alpha2}//[22\bar{4}\bar{3}]_{\omega o}, (0002)_{\alpha2}//(01\bar{1}2)_{\omega o}$. The other ORs observed are subsets of these two ORs. The edge-to-edge matching model is applied to predict the possible ORs between the ordered α_2 and ω_o phases based on the calculated close-packed planes of the two phases. The simulation results agree well with the experimental results.

Keywords: Titanium aluminides; Phase transformation; TEM; Orientation relationship; Edge-to-edge matching

1. Introduction

High Nb-containing TiAl (Nb-TiAl) alloys are considered to be promising high temperature structural materials for use in aerospace engineering [1–4]. However, due to the high concentration of Nb in these materials, the β_o phase (B2 structure, space group: $Pm\bar{3}m$), which results from ordering of the β phase (A2 structure, space group: $Im\bar{3}m$), is usually retained as a constituent of the as-cast microstructure. Recent publications revealed that the high-temperature β phase is beneficial for the thermomechanical processing of TiAl alloys and some alloys are modified to possess a microstructure containing more β_o phase to improve workability [5–7]. However, the β_o phase and the coexisting ordered ω phases inside deteriorate the room temperature ductility of the alloys, because these areas are commonly observed to be the source of cracks and thus they are not desirable [8–10]. As a result, efforts have been made to eliminate the $\beta_o(\omega)$ phase by thermomechancial processing or heat treatments. In recent years, the ordered ω phases in high Nb-TiAl alloys have garnered increasing attention due to their variable structures and morphologies, which can be induced by different heat treatment processes [10–20]. Commonly, the designation ω is restricted to the disordered ω phase (space group P6/mmm) in Ti based alloys. In intermetallics alloys, phases with similar crystal structures but with two or more differently occupied atom sites are designated ω-related phases or ordered ω phases. These phases include the trigonal ω' and ω'' phases as well as the hexagonal ω_o in the $B8_2$ structure [11]. Among the different ordered variants, the ω_o phase is the most commonly reported phase in research literature [13–18], in which three Wykoff positions (i.e. 2a, 2c and 2d) are occupied by proportional Ti, Al and Nb atoms. In the disordered ω phase, the 1a and 2d Wykoff positions are occupied by the same type of atom [11]. On the other hand, the α_2-Ti_3Al phase in the $D0_{19}$ structure is a main phase in TiAl intermetallics, in which the Wykoff positions 2c and 6 h are occupied by Al and Ti atoms, respectively. In disordered α phase, the 2c positions are occupied by the same type of atom. To better understand the phases considered in this study, the crystal structures of the ordered phases are compared with those of the corresponding disordered phases, as shown in Fig. 1 and Table 1.

Numerous studies have demonstrated that the ω_o phase is stable at intermediate temperatures (700–900 °C) in high Nb-TiAl alloys. However, these studies have mainly focused on the interconversion between the ordered ω phases and the parent β_o phase [10–16] or the α_2 to β_o phase transformation [21–24]; few reports have concentrated on the relationship between the ordered ω phases and the α_2 phase. Recently, Huang et al. [25–29] claimed that after annealing

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http://dx.doi.org/10.1016/j.actamat.2015.03.025
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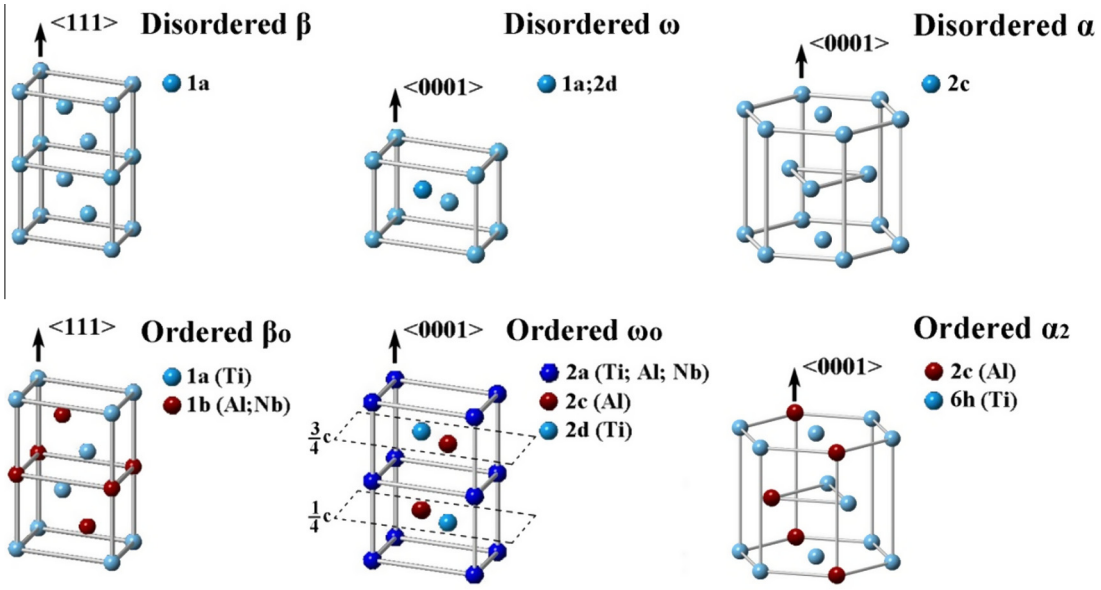

Fig. 1. Crystal structures and Wyckoff positions of the disordered (β, ω and α) and ordered (β_o, ω_o and α_2) phases.

Table 1. Crystal parameters of the disordered (β, ω and α) and ordered (β_o, ω_o and α_2) phases.

Phase	Pearson symbol	Strukturbericht designation	Space group	Wyckoff position	Coordinate x	Coordinate y	Coordinate z	Lattice parameters (nm)	c/a
ω-Ti	hP3		P6/mmm	1a 2d	0 0.3333	0 0.6667	0 0.5	$a = 0.463$ $c = 0.281$	0.61 [48]
ω_o	hP6	$B8_2$	$P6_3/mmc$	2a 2c 2d	0 0.3333 0.3333	0 0.6667 0.6667	0 0.25 0.75	$a = 0.459$ $c = 0.556$	1.21
α-Ti	hP2	A3	$P6_3/mmc$	2c	0.3333	0.6667	0.25	$a = 0.291$ $c = 0.467$	1.60 [49]
α_2	hP8	$D0_{19}$	$P6_3/mmc$	2c	0.3333	0.6667	0.25	$a = 0.579$ $c = 0.461$	0.80

certain high Nb-TiAl alloys at intermediate temperatures for long periods, the $\beta_o(\omega)$ precipitated along the α_2 laths or at parts of the lamellar structures, which are composed of closely spaced α_2/γ laths. The orientation relationship (OR) can be expressed as follows: $\langle 11\bar{2}0\rangle_{\alpha 2}//\langle 111\rangle_{\beta o}//\langle 0001\rangle_{\omega}$; $\{0001\}_{\alpha 2}//\{110\}_{\beta o}//\{11\bar{2}0\}_{\omega}$. Bystrzanowski et al. [17] observed that the applied stress could enhance the ω_o precipitation and suspected that the observed ω_o particles were directly derived from the α_2 phase. The ω_o phase is generally observed within the β_o phase without direct contact with other phases, which is most likely the reason for the limited number of investigations on the α_2 to ω_o phase transformation.

In contrast, some reports have focused on the ORs between disordered ω and α phases [30–41], mostly for Zr-based metals. However, the results of these studies have shown to be controversial. Early studies by Usikov et al. [30] indicated that the $\alpha \rightarrow \omega$ transformation in pure Ti and Zr happens via the unstable β phase, i.e., via the transformation path $\alpha \rightarrow \beta \rightarrow \omega$. Because the $\alpha \rightarrow \beta$ and $\beta \rightarrow \omega$ transformations are both clearly understood with respect to their crystallographic characters, the ORs between these two phases can be deduced to be as follows:

$$\langle 11\bar{2}0\rangle_{\alpha}//\langle 0001\rangle_{\omega},\ \{0001\}_{\alpha}//\{11\bar{2}0\}_{\omega} \qquad \text{(ORI)}$$

and

$$\langle 11\bar{2}0\rangle_{\alpha}//\langle 10\bar{1}1\rangle_{\omega}//\{0001\}_{\alpha}//\{01\bar{1}1\}_{\omega} \qquad \text{(ORII)}$$

More recently, experimental evidence of an $\alpha \rightarrow \beta \rightarrow \omega$ transformation was reported by Vohra et al. [31] and Gupta et al. [32]. Nevertheless, neither of these studies could completely dismiss the pre-existing β phase. Song et al. [35] reported a new OR in Zr that is different from the two abovementioned ORs:

$$\langle 10\bar{1}0\rangle_{\alpha}//\langle 11\bar{2}\bar{3}\rangle_{\omega}//\{0001\}_{\alpha}//\{10\bar{1}1\}_{\omega} \qquad \text{(ORIII)}$$

However, Jyoti et al. [36–37] proved that ORIII was a subset of ORII, claiming that the $\alpha \rightarrow \omega$ transformation could be directly achieved without the precipitation of an intermediate β phase. Other investigations have indicated that the $\alpha \rightarrow \omega$ transformation could be realized through heat treatment or shear strain [39–41]. In summary, the aforementioned studies have mainly focused on displacive/diffusionless phase transformations, whereas few works have attempted to elucidate a diffusion-controlled mechanism.

Qiu et al. [39] reported that the plate-shaped, athermal ω phase nucleates at the α' martensite plate, using the edge-to-edge matching (E2EM) model to predict the ORs between